Yield and Failure Behavior Investigated for Cross-Linked Phenolic Resins Using Molecular Dynamics

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Molecular dynamics simulations were conducted to fundamentally evaluate the yield and failure behavior of cross-linked phenolic resins at temperatures below the glass transition. Yield stress was investigated at various temperatures, strain rates, and degrees of cross-linking. The onset of non-linear behavior in the cross-linked phenolic structures was caused by localized irreversible molecular rearrangements through the rotation of methylene linkers followed by the formation or annihilation of neighboring hydrogen bonds. The yield stress results, with respect to temperature and strain rate, could be fit by existing models used to describe yield behavior of amorphous glasses. The degree of cross-linking only indirectly influences the maximum yield stress through its influence on glass transition temperature (Tg), however there is a strong relationship between the degree of cross-linking and the failure mechanism. Low cross-linked samples were able to separate through void formation, whereas the highly cross-linked structures exhibited bond scission.